

Carbazole-2-carbonitrile, 5,6,7,8-tetrahydro-1-methyl-
73771-63-8 | DTXSID50224153

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.64 days

Global applicability domain: Outside

Local applicability domain index: 2.88e-01

Confidence level: 8.76e-01

Nearest Neighbors from the Training Set

Image not found

1-Methyl-2-propylbenzene

Measured: 12.5

Predicted: 3.17

Image not found

9-Ethyl-9H-fluorene

Measured: 2330

Predicted: N/A

Image not found

3-Ethyltoluene

Measured: 12.5

Predicted: 3.26

Image not found

5-Methylindan

Measured: 4.93

Predicted: 2.25

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1,3-Dimethyl-4-ethylbenzene

Measured: 24.3

Predicted: 3.89